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FILE COVERS 1907 - 31 Aug 2004  VOL 141 ISS 10
FILE LAST UPDATED: 30 Aug 2004  (20040830/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


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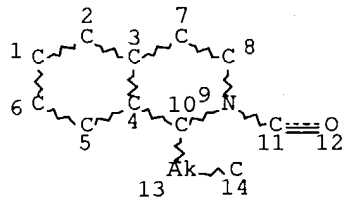


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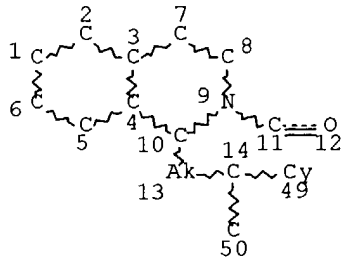

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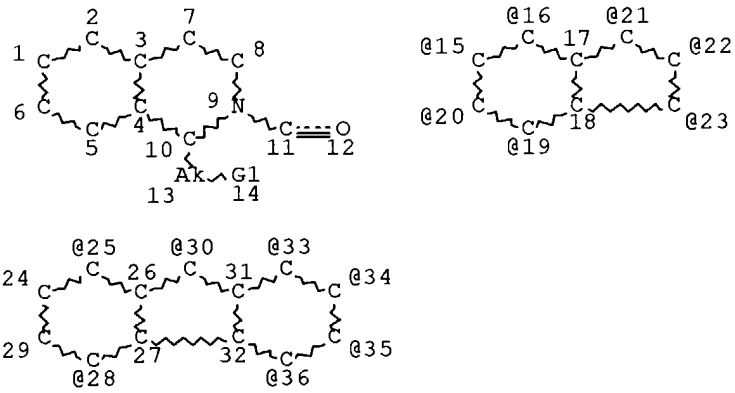

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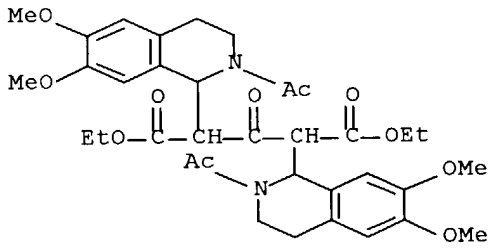
=> d ibib abs hitstr l25 1-4

L25 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:335639 HCAPLUS Full-text
DOCUMENT NUMBER: 125:58291
TITLE: Reaction of 3,4-dihydroisoquinolines with 1,3-dicarbonyl compounds and carboxylic acid chlorides. Novel synthesis of 2-(2-acyltetrahydroisoquinolin-1-yl)-1,3-dicarbonyl compounds
AUTHOR(S): Akhrem, A. A.; Borisov, E. V.; Chernov, Yu. G.
CORPORATE SOURCE: Inst. Bioorg. Khim., Akad. Nauk Respub. Belarus, Minsk, Belarus
SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(11), 1715-1720
CODEN: ZORKAE; ISSN: 0514-7492
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

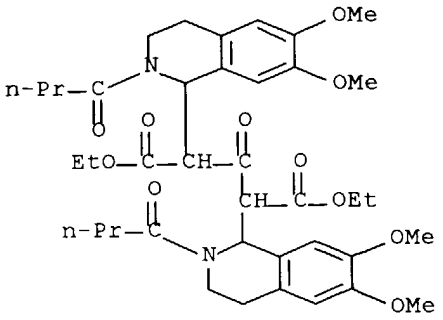
AB Reaction of 3,4-dihydroisoquinolines with carboxylic acid chlorides and 1,3-dicarbonyl compds. (1,3-diketones and β-keto esters) produced a series of 2-(2-acyltetrahydroisoquinolin-1-yl)-1,3-dicarbonyl compds. The stereochem. and tautomerism of the products were discussed.

IT **175983-15-0P 175983-16-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-(2-acyltetrahydroisoquinolin-1-yl)-1,3-dicarbonyl compds. by reaction of 3,4-dihydroisoquinolines with 1,3-dicarbonyl compds. and carboxylic acid chlorides)

RN 175983-15-0 HCAPLUS
CN Pentanedioic acid, 2,4-bis(2-acetyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl)-3-oxo-, diethyl ester (9CI) (CA INDEX NAME)



RN 175983-16-1 HCAPLUS
CN Pentanedioic acid, 3-oxo-2,4-bis[1,2,3,4-tetrahydro-6,7-dimethoxy-2-(1-oxobutyl)-1-isoquinolinyl]-, diethyl ester (9CI) (CA INDEX NAME)



L25 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:162169 HCAPLUS Full-text
DOCUMENT NUMBER: 124:316960
TITLE: Reaction of 3,4-dihydroisoquinolines with β-keto ester enol acylates
AUTHOR(S): Akhrem, A. A.; Borisov, E. V.; Chernov, Yu. G.
CORPORATE SOURCE: Inst. Bioorg. Khim., Minsk, Belarus
SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(8), 1241-5
CODEN: ZORKAE; ISSN: 0514-7492
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
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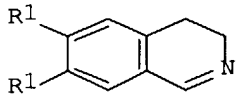

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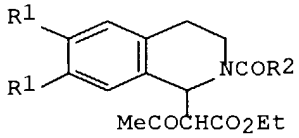

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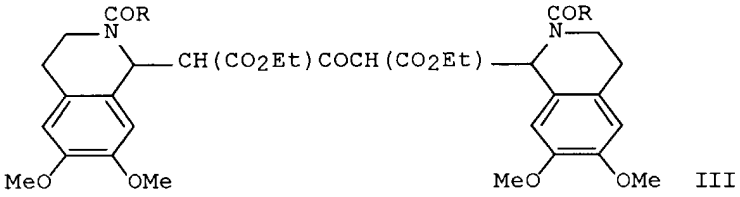

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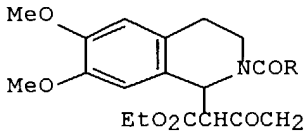


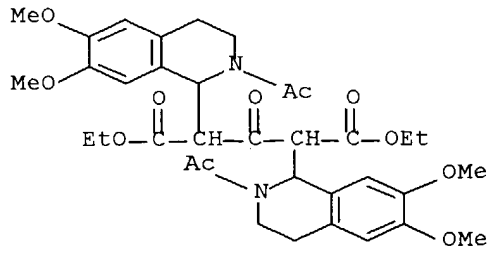
IV

AB Dihydroisoquinolines I (R1 = H, MeO) reacted with R2CO2CMe:CHCO2Et (R2 = Ph, Me) to give adducts II. I (R1 = MeO) reacted with EtO2CCH2C(OCOR):CHCO2Et (R = Me, Pr) to give adducts III and IV.

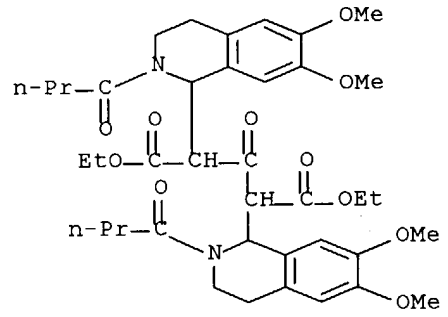
IT **175983-15-0P 175983-16-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 175983-15-0 HCAPLUS

CN Pentanedioic acid, 2,4-bis(2-acetyl-1,2,3,4-tetrahydro-6,7-dimethoxy-1-isoquinolinyl)-3-oxo-, diethyl ester (9CI) (CA INDEX NAME)



RN 175983-16-1 HCAPLUS
CN Pentanedioic acid, 3-oxo-2,4-bis[1,2,3,4-tetrahydro-6,7-dimethoxy-2-(1-oxobutyl)-1-isoquinolinyl]-, diethyl ester (9CI) (CA INDEX NAME)

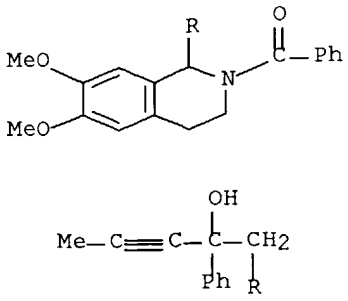


L25 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:516903 HCAPLUS Full-text
DOCUMENT NUMBER: 67:116903
TITLE: Reaction of vinyl bromide and substituted vinyl bromides with lithium in tetrahydrofuran with formation of lithium acetylides
AUTHOR(S): Schoepf, Clemens; Strauss, Hans J.; Hoehn, Monika; Hutzler, Anneliese
CORPORATE SOURCE: Tech. Hochsch., Darmstadt, Fed. Rep. Ger.
SOURCE: Monatshefte fuer Chemie (1967), 98(4), 1274-309
CODEN: MOCHAP
DOCUMENT TYPE: Journal
LANGUAGE: German

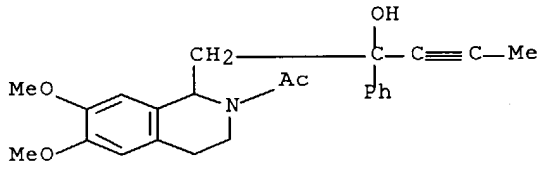
AB Treatment of 2-bromopropene and 2-bromo-1-butene with Li in boiling tetrahydrofuran (THF) led to Li acetylides, instead of the expected Li alkenes. The major products were the free alkene and LiBr, with a smaller amount of LiH. Similarly, with vinyl bromide the acetylide was formed together with LiH, while Li vinyl was not found. cis-1-Bromo-1-butene also gave the acetylide. In THF the formation of Li acetylide from 2-bromopropene proceeded at -65°, while in Et2O reflux temps. were required. Acetylides were also obtained from PhC.tplbond.CH and 1-octyne, while very little reaction was observed with HC.tplbond.CH. The mechanism of acetylide formation is discussed.

IT **16557-12-3P 16557-17-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16557-12-3 HCAPLUS
CN 1-Isoquinolineethanol, 2-benzoyl-1,2,3,4-tetrahydro-6,7-dimethoxy-α-phenyl-α-1-propynyl- (8CI) (CA INDEX NAME)



RN 16557-17-8 HCAPLUS
CN 1-Isoquinolineethanol, 2-acetyl-1,2,3,4-tetrahydro-6,7-dimethoxy-α-phenyl-α-1-propynyl- (8CI) (CA INDEX NAME)



L25 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1964:418195 HCAPLUS Full-text
DOCUMENT NUMBER: 61:18195
ORIGINAL REFERENCE NO.: 61:3079h,3080a-h
TITLE: Quinolizine derivatives
INVENTOR(S): Schoepf, Clemens; Klug, Rudolf
PATENT ASSIGNEE(S): E. Merck, A.G.
SOURCE: 8 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3132147		19640505	US	
BE 632428			BE	
FR 1431659			FR	
GB 977725			GB	
PRIORITY APPLN. INFO.:			DE	19610619

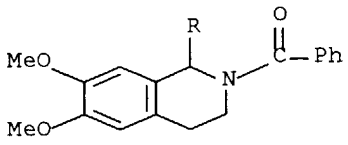
OTHER SOURCE(S): CASREACT 61:18195
GI For diagram(s), see printed CA Issue.
AB Vinyl bromide (105 g.) in 240 ml. tetrahydrofuran (THF) is treated with 24 g. Mg. in 210 ml. THF to form the Grignard compound, an addnl. 350 ml. THF added, 60 g. 1-phenacyl-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline added with stirring and cooling, the mixture kept at 35° 4.5 hrs. and decomposed with ice-cooling with 250 ml. of saturated NH4Cl, the THF layer separated, and the residue extracted with CH2Cl2 to give, from the combined organic solvents, 68% [(6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)methyl](phenyl)(vinyl)carbinol (I), m. 126-8° (iso-PrOH); HCl salt m. 210-12° (EtOH); HBr salt m. 215-16° (EtOH). A solution of 14.8 g. I.HCl in 61 ml. SOCl2 is kept at room temperature 16 hrs. and the SOCl2

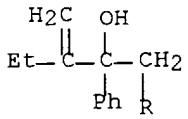
evaporated to yield 62.6% 1-(6,7-dimethoxy-1,2,3,4- tetrahydro-1-isoquinolyl-2-phenyl-4-chloro-2-butene-HCl (II), m. 163-4° (EtOH). II (10 g.) is agitated with 45 ml. CH2Cl2 and 25 ml. 2N NaOH 15 min.; the combined organic solvents give 72% 1,4,6,7-tetrahydro-9,10-dimethoxy-2-phenyl-11bH-benzo[a]quinolizine (III), m. 123-5° (iso-PrOH); HCl salt m. 200-1°; HBr salt m. 214-16°. A solution of 440 mg. III.HCl in 22 ml. MeOH and 1 ml. 2N NaOH is hydrogenated at room temperature under normal pressure in the presence of Raney Ni, the catalyst filtered off, the solvent evaporated, the residue mixed with 5 ml. H2O and extracted with 4 portions CH2Cl2, and the exts. evaporated to give 75% 1,2,3,4,6,7-hexahydro-9,10-dimethoxy-2-phenyl-11bH- benzo[a]quinolizine, m. 89-90° (iso-PrOH); HCl salt m. 229-30°; HBr salt m. 202-4° (decompn). A solution of 60 g. 6,7-dimethoxy-3,4-dihydroisoquinoline in 700 ml. H2O and 250 ml. MeOH are added to a citrate-buffered aqueous solution (pH 4.6) and mixed with 60 g. of BzCH2CO2H in 200 ml. 2 N NaOH, the volume made up to 2 l. with H2O and MeOH, the mixture kept 20 hrs. at pH 4.6 and 25°, and 250 ml. 2N NaOH added to give 88% 1-phenacyl - 6,7 - dimethoxy - 1,2,3,4 - tetrahydroisoquinoline, m. 138-9° (Me2CO). The following were similarly prepd: bis[(2-benzoyl-6,7-dimethoxy - 1,2,3,4 - tetrahydro - 1 - isoquinolyl)methyl](1-buten-2-yl)carbinol (IV), m. 225-7° (HCONMe2-EtOH); bis [(6,7 - dimethoxy - 1,2,3,4 - tetrahydro - 1 - isoquinolyl)methyl] -[1-buten-2-yl]carbinol, m. 126-8° (di-HCl salt m. 250-2°); 1-(6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl) - 2 - [(6,7 - dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)methyl] - 3- chloromethyl-2-pentene-2HCl, m. 230-3°; α,α'-bis(2- benzoyl-6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)acetone-2HBr, m. 204-5° (meso form m. 178-80°; dibenzoyl derivative m. 198°); bis[(2-benzoyl-6,7-dimethoxy-1,2,3,4-tetrahydro- 1-isoquinolyl)methyl] (1 - buten - 2-yl)carbinol; bis [(6,7-dimethoxy- 1,2,3,4-tetrahydro- 1-isoquinolylmethyl] (1-buten-2-yl)carbinol; 2-dehydroemetine(3-ethyl-9,10-dimethoxy-1,6,7,11b-tetrahydro-2-[(6,7- dimethoxy - 1,2,3,4- tetrahydro-1-isoquinolyl)methyl]-4H- benzo[a]quinolizine, m. 112-14° and 194-5° (di-HCl salt m. 248-50°); α,α'-bis(N-benzoyl-6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)acetone, m. 178-80°; α,α'-bis (6,7-dimethoxy- 1,2,3,4-tetrahydro-1-isoquinolyl)acetone, m. 144-5° (di-HCl salt m. 193-5°; methanesulfonate m. 173-4°); α,α'-bis(2-acetyl-6,7-dimethoxy-1,2,3,4-tetrahydro-1-isoquinolyl)acetone, m. 191-2°; bis[(6,7-dimethoxy-1,2,3,4- tetrahydro-1-isoquinolyl)methyl]-1-buten-2-ylcarbinol-2HCl, m. 193-201°; 9,10-dimethoxy-1,6,7,11b-tetrahydro-2-heptyl-4H-benzo [a] quinolizidine; 1-phenacyl-2-benzoyl - 6,7 - dimethoxy-1,2,3,4- tetrahydroisoquinoline, m. 190-3°; [(2-benzoyl-6,7-dimethoxy - 1,2,3,4 - tetrahydro - 1 - isoquinolyl)methyl]-(phenyl)(1-buten-2- yl)carbinol, m. 164-6° (AcOH ester); (6,7-dimethoxy-1,2,3,4- tetrahydro-1-isoquinolyl)-3-phenyl-2-ethyl - 1-buten-3-ol-HCl, m. 191-3° (iso-PrOH) [free base m. 115-16° (iso-PrOH-H2O)]; 1,4,6,7-tetrahydro-9,10-dimethoxy-2-phenyl-3-ethyl-11bH- benzo[a]quinolizine-HCl, m. 209-12° (iso-PrOH) (perchlorate m. 198-9°); 3-ethyl-9,10-diethoxy-1,6,7,11b-tetrahydro-2-[(1,2,3,4- tetrahydro-6,7 - diethoxy - 1 - isoquinolyl)methyl]-4H-benzo [a] quinolizine-2HCl; 3-ethyl-9,10-diethyl-1,6,7,11b-tetrahydro-2-[(1,2,3,4 - tetrahydro - 6,7 - diethyl - 1 - isoquinolyl)-methyl]-4H-benzo[a] quinolizine -2HCl; 1,4,6,7- tetrahydro-2-phenyl-11bH-benzo [a] quinolizine-2HCl; 1,2,3,4,6,7-hexahydro-2-phenyl- 11bH-benzo [a] quinolizine; 1,2,3,4,6,7-hexahydro-9-chloro-2-phenyl- 11bH-benzo[a] quinolizine (V); 3-ethyl-9,10-methylenedioxy - 1,6,7,11b - tetrahydro - 2 - [(1,2,3,4 - tetrahydro-6,7-methylenedioxy - 1 - isoquinolyl)methyl] - 4H - benzo[a] quinolizine; α,α'-bis(2-acetyl-6,7-methylenedioxy- 1,2,3,4-tetrahydro-1-isoquinolyl)acetone-2HBr, m. 243-7° 188-9° (decomposition).

IT **96377-86-5**, 1-Isoquinolineethanol, 2-benzoyl-α-(1-ethylvinyl)-1,2,3,4-tetra-hydro-6,7-dimethoxy-α-phenyl-
(preparation of)

RN 96377-86-5 HCAPLUS

CN 1-Isoquinolineethanol, 2-benzoyl-α-(1-ethylvinyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-α-phenyl- (7CI) (CA INDEX NAME)





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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L26 1 L24

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=> d all l26

L26 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN
AN CA61:3079h CAOLD
TI 8-aminoquinoline
AU Korzunov, N. P.
DT Patent
TI quinolizine derivs.
AU Schoepf, Clemens; Klug, R.
PA Merck, E., A.-G.
DT Patent

	PATENT NO.	KIND	DATE
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     BE 632428
     FR 1431659
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IT   2649-50-5   4914-30-1  21319-81-3  47728-07-4  66833-37-2  94910-05-1
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USE THE FILE COMMAND TO CHANGE TO THE CORRECT FILE.

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'HITRN' IS NOT A VALID FIELD CODE FOR FILE 'CAOLD'
ENTER DISPLAY CODE (IT) OR ?:rn
E1 THROUGH E25 ASSIGNED

=> select hit rn l26
ENTER ANSWER NUMBER OR RANGE (1-):.
E26 THROUGH E26 ASSIGNED

=> fil reg
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STRUCTURE FILE UPDATES:   30 AUG 2004  HIGHEST RN 736108-36-4
DICTIONARY FILE UPDATES:  30 AUG 2004  HIGHEST RN 736108-36-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L27          1 96377-86-5/RN

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L27  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
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RN **96377-86-5** REGISTRY

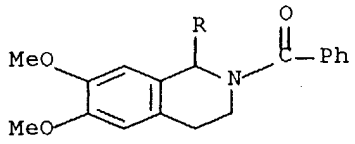
CN 1-Isoquinolineethanol, 2-benzoyl-α-(1-ethylvinyl)-1,2,3,4-tetrahydro-6,7-dimethoxy-α-phenyl- (7CI) (CA INDEX NAME)

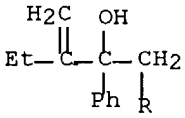
MF C30 H33 N O4

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data)

DT.CA CAplus document type: Patent

RL.P Roles from patents: NORL (No role in record)





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 61:18195